

Nortriptyline M(di-HO)

Inchi:	InChI=1S/C18H19NO2/c19-9-1-2-18-16-7-5-14(20)10-12(16)3-4-13-11-15(21)6-8-17(13)
InchiKey:	LNWCYWATZJEOKC-UHFFFAOYSA-N
Formula:	C18H19NO2
SMILES:	NCCC=C1c2ccc(O)cc2CCc2cc(O)ccc21
Mol. weight [g/mol]:	281.35

Physical Properties

Property code	Value	Unit	Source
gf	177.37	kJ/mol	Joback Method
hf	-116.39	kJ/mol	Joback Method
hfus	43.83	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.977		Crippen Method
mcvol	223.520	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinsol	2800.00		NIST Webbook
tb	926.38	K	Joback Method
tc	1186.71	K	Joback Method
tf	709.74	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.08	J/molxK	926.38	Joback Method
cpg	713.69	J/molxK	969.77	Joback Method
cpg	729.63	J/molxK	1013.16	Joback Method
cpg	746.21	J/molxK	1056.54	Joback Method
cpg	763.73	J/molxK	1099.93	Joback Method
cpg	782.48	J/molxK	1143.32	Joback Method
cpg	802.77	J/molxK	1186.71	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R213391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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